

# Cluster superheating during nonisothermal nucleation.

Perevoshchikov E.E.<sup>1,2,@</sup> and Zhukhovitskii D.I.<sup>2</sup>

<sup>1</sup> Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, 141701, Russia

<sup>2</sup> Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow, 125412, Russia

@ dmr@ihed.ras.ru

We investigate stationary vapor–liquid nucleation in a Lennard–Jones system under isothermal and nonisothermal conditions using molecular dynamics with a steady-state removal/reinjection protocol for post-critical clusters and monomers. In nonisothermal runs, monomers are weakly thermostatted while larger clusters evolve freely. A robust temperature–size structure emerges [1]. At lower supersaturation  $S$ , subcritical clusters start slightly cooler than the vapor and then warm up, so that near-critical nuclei are already superheated relative to monomers. At higher supersaturation the temperature–size curve becomes monotonically increasing. This superheating feeds back on cluster populations and on the compressibility factor of the vapor, and thereby on the nucleation flux. It is shown that nonisothermal heating lowers the compressibility factor by roughly a factor of 1.6 compared with isothermal dynamics. Measured nucleation rates versus supersaturation agree with a two parameter nucleation model augmented by a nonisothermal diffusion correction [1], yielding about an order-of-magnitude reduction relative to isothermal kinetics. Critical sizes inferred from the nucleation theorem match theory for isothermal conditions, but exceed predictions in nonisothermal runs, consistent with persistent superheating of near-critical nuclei. Overall, the results establish cluster temperature as a controlling state variable: resolving the temperature–size dependency is essential to determine the true supersaturation, vapor nonideality, and the resulting nonisothermal nucleation rate.

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